

Information entropy as a measure of the quality of a nuclear density distribution

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February 9, 2008

Abstract

The information entropy of a nuclear density distribution is calculated for a number of nuclei. Various phenomenological models for the density distribution using different geometry are employed. Nuclear densities calculated within various microscopic mean field approaches are also employed. It turns out that the entropy increases on going from crude phenomenological models to more sophisticated (microscopic) ones. It is concluded that the larger the information entropy, the better the quality of the nuclear density distribution. An alternative approach is also examined: the net information content i.e. the sum of information entropies in position and momentum space $S_r + S_k$. It is indicated that $S_r + S_k$ is a maximum, when the best fit to experimental data of the density and momentum distributions is attained.

1 Introduction

Information-theoretic methods have started recently to be important for the study of quantum mechanical systems, [1, 2, 3, 4, 5, 6, 7, 8, 9] mainly through the application of

the maximum entropy principle (MEP) [10, 11]. This is done by employing a suitably defined quantum entropy that measures the lack of information associated with the distribution of a quantum state over a given known basis. The MEP provides the least biased description consistent with the available relevant information.

In [12] Ghosh, Berkowitz and Parr (GBP) defined, within the ground-state density functional framework, several local quantities of thermodynamic-like character in order to characterize a non-homogenous many-electron system. Specifically, they introduced the concept of a local temperature corresponding to the electronic motion and an information entropy \mathcal{S} associated with the electron distribution of an atomic system. An interesting result [13] is that \mathcal{S} increases with the quality of the wavefunction.

Gadre and Bendale (GB) [5, 6] investigated a different MEP procedure for atomic systems. They studied basis-set effects on the entropy sum $\mathcal{S}_r + \mathcal{S}_k$, where \mathcal{S}_r is the position-space entropy and \mathcal{S}_k is the momentum-space entropy. They found that this sum increases with the basis-set quality, so that $\mathcal{S}_r + \mathcal{S}_k$ can be used as a measure of the quality of the electronic density distribution.

A recent attempt to apply information theory to nuclear systems is ref. [9] where the sum $\mathcal{S}_r + \mathcal{S}_k$ has been calculated employing two phenomenological models for the nucleus. An interesting result was that the same functional form $\mathcal{S} = aN + bN \ln N$ for the entropy as function of the particle number N (electrons or nucleons) holds approximately for atomic and nuclear systems.

The nucleon distributions in nuclei is of fundamental importance in our understanding of nuclear properties. There are several functional forms which are used for the description of the nuclear distributions. Their parameters are usually fitted to the available empirical data for the mean square radii. Moreover, density dependent Hartree-Fock (DDHF) [14] calculations with Skyrme or Gogny type interactions or the relativistic mean field (RMF) [15] calculations yield fairly reliable ground state nuclear properties including the densities.

In the present paper we attempt to apply the approaches of GBP and GB as a criterion of the quality of nuclear density distributions derived according to various nuclear models. We hope that this will lead to a method to choose the best nuclear density in different situations of practical interest, although as the models increase in sophistication, it turns out that the value of \mathcal{S} stops to increase and tends to saturation.

The paper is organized as follows: In section 2 we present the formalism of the information entropy according to GBP. In section 3 the numerical results are shown and discussed. In section 4 an alternative approach (GB) i.e. the sum $\mathcal{S}_r + \mathcal{S}_k$ is discussed. In section 5 numerical results for GB are presented and finally section 6 summarises our conclusions.

2 The formalism of information entropy in phase-space

In [12, 13] Ghosh, Berkowitz and Parr introduced a phase-space distribution $f(\bar{r}, \bar{p})$ associated with the ground-state density $\rho(\bar{r})$ of a N-electron system. The distribution $f(\bar{r}, \bar{p})$ satisfies the relations

$$\begin{aligned}\rho(\bar{r}) &= \int d\bar{p} f(\bar{r}, \bar{p}) \\ \int d\bar{r} \rho(\bar{r}) &= N \\ t(\bar{r}; \rho) &= \frac{1}{2} \int d\bar{p} p^2 f(\bar{r}, \bar{p})\end{aligned}\tag{1}$$

where $t(\bar{r}; \rho)$ is the kinetic energy density.

Then, they defined an entropy density $s(\bar{r})$ and entropy \mathcal{S} associated with the electron density $\rho(\bar{r})$ in terms of $f(\bar{r}, \bar{p})$

$$s(\bar{r}) = -k \int d\bar{p} f(\ln f - 1)\tag{2}$$

$$\mathcal{S} = \int d\bar{r} s(\bar{r})\tag{3}$$

and obtained the most probable distribution $f(\bar{r}, \bar{p})$ by maximizing this functional subject to the constraints of correct density $\rho(\bar{r})$ and correct kinetic energy density $t(\bar{r}; \rho)$.

The phase-space distribution function $f(\bar{r}, \bar{p})$ is given by a local Maxwell-Boltzmann distribution law:

$$f(\bar{r}, \bar{p}) = (\beta(\bar{r})/2\pi)^{3/2} \rho(\bar{r}) \exp(-\frac{1}{2} p^2 \beta(\bar{r}))\tag{4}$$

where $\beta(\bar{r}) = 1/kT(\bar{r})$. The local temperature $T(\bar{r})$ is defined by the ideal-gas expression for the kinetic energy:

$$t(\bar{r}; \rho) = (3/2) \rho(\bar{r}) kT(\bar{r})\tag{5}$$

Substituting eq. (4) into eq. (3) yields the Sackur-Tetrode equation [12] for the entropy:

$$\mathcal{S} = k \int \rho \left[\frac{5}{2} - \ln \rho + \frac{3}{2} \ln(2\pi kT) \right] d\bar{r}\tag{6}$$

The entropy density can also be rewritten in the form:

$$s(r) = \frac{3}{2} k \rho [\ln(t/t_{TF}) + c]\tag{7}$$

where $t_{TF} = c_k \rho^{5/3}$ is the Thomas-Fermi kinetic energy density. For convenience, \bar{r} and ρ are dropped from the argument of t . The constants c and c_k are given by:

$$c = \frac{5}{3} + \ln(4\pi c_k/3), \quad c_k = \frac{3}{10}(3\pi^2)^{2/3} \quad (8)$$

In [13] it was found that the entropy increases with the quality of the electron wavefunction. As stated in [12], one can omit all considerations for $f(\bar{r}, \bar{p})$ and simply postulate the existence of (7) and (3). Thus we postulate these expressions for another many fermion system i.e. the nucleus. In the present article, we attempt to answer the question: Does this \mathcal{S} increase with the quality of nuclear density distribution as well? It turns out that the answer is yes. In other words, we derive a criterion to assess the quality of a nuclear density distribution $\rho(r)$ by observing an increase of \mathcal{S} on going from crude to more sophisticated models of the nucleus.

3 Numerical results for \mathcal{S}

It is well known that the kinetic energy density t is not uniquely defined. Thus, there are various expressions for this quantity [13]:

$$t_1 = \frac{1}{8} \sum_i \frac{|\nabla \rho_i|^2}{\rho_i} - \frac{1}{4} \nabla^2 \rho \quad (9)$$

$$t_2 = \frac{1}{8} \sum_i \frac{|\nabla \rho_i|^2}{\rho_i} \quad (10)$$

$$t_3 = \frac{1}{8} \sum_i \frac{|\nabla \rho_i|^2}{\rho_i} - \frac{1}{8} \nabla^2 \rho \quad (11)$$

For simplicity we have chosen the Thomas-Fermi-Weizsäcker kinetic energy expression [13]:

$$t_{TFW} = t_{TF} + \frac{1}{72} \frac{|\nabla \rho|^2}{\rho} \quad (12)$$

This choice allows us to use various functional forms of the density distributions, where no knowledge of the contribution to the density from each orbit is necessary. This is also corroborated indirectly by the fact that in [13], using (12), there is not a single exception to the trend of the information entropy to increase as the quality of the electron wavefunction increases.

We calculate \mathcal{S} employing as an input several nuclear (matter) density distributions:

1) Uniform (UN) specified by the well-known rule: $R = r_0 A^{-1/3}$

$$\rho(r) = \begin{cases} \rho_0 & r \leq R \\ 0 & r > R \end{cases} \quad (13)$$

2) Trapezoidal (TR) [16]:

$$\rho(r) = \begin{cases} \rho_0 & r < c - z \\ \rho_0(c + z - r)/2z & c - z \leq r \leq c + z \\ 0 & r > c + z \end{cases} \quad (14)$$

where c is the half-way radius and $2z$ is the width of the surface region.

3) Two parameter Fermi (FM) [17]:

$$\rho(r) = \frac{\rho_0}{1 + \exp\left(\frac{r-R}{\alpha}\right)} \quad (15)$$

For the half density radius R , instead of the well known expression $R = r_0 A^{-1/3}$ an expression with an A -dependent radius parameter $r_0 = r_0(A)$ is used, which results from the solution of an algebraic third order equation for the normalization of the density [17]:

$$r_0(A) = \left(\frac{1}{2^{1/3}}\right) r_0 \left\{ \left[1 + \left[1 + \frac{4}{27} \left(\frac{\pi\alpha}{r_0 A^{1/3}} \right)^6 \right]^{1/2} \right]^{1/3} + \left[1 - \left[1 + \frac{4}{27} \left(\frac{\pi\alpha}{r_0 A^{1/3}} \right)^6 \right]^{1/2} \right]^{1/3} \right\} \quad (16)$$

where

$$r_0 = (3/4\pi\rho_0)^{1/3} \quad (17)$$

It is noted that the same expression for the half density radius has also been used for the trapezoidal distribution ($c = R$), where $\pi\alpha = z$. In both cases the parameters were determined by a global least squares procedure to the available experimental rms radii.

4) Harmonic Oscillator (HO) Shell Model, specified by the rule : $\hbar\omega = 41A^{-1/3}$

5) Semiphenomenological single-particle density (SP-D) of Gambhir and Patil [18, 19, 20, 21]. We use the expression of ref. [18]

$$\rho_i(r) = \frac{\rho_i^0}{1 + \beta_i \left[1 + \left(\frac{r}{R + a_i} \right)^2 \right]^{\alpha_i} \left[e^{\frac{(r-R)}{a_i}} + e^{\frac{-(r+R)}{a_i}} \right]} \quad (18)$$

where

$$\beta_i = [1 + (\frac{R}{R + a_i})^2]^{-\alpha_i}$$

(in order to identify R with the half-way radius), the index $i = n$ (for neutrons) or p (for protons), R is a measure of the size of the nucleus and a_i and α_i are given in terms of the separation energy ϵ_i of the last particle (neutron or proton) through:

$$a_i = \frac{\hbar}{2\sqrt{2m\epsilon_i}}; \quad (19)$$

$$\alpha_i = \frac{q}{\hbar} \sqrt{\frac{m}{2\epsilon_i}} + 1 \quad (20)$$

Here m is the nucleon mass and $q = 0$ for neutrons and $q = Z - 1$ for protons.

The above $\rho_i(r)$ correctly incorporates the following two important physical requirements:

- a) The small r ($r \rightarrow 0$) behaviour which implies that the density contains only even powers of r .
- b) The asymptotic behaviour

$$\rho_i(r) \rightarrow r^{-2\alpha_i} \exp(-r/a_i) \quad (r \rightarrow \infty) \quad (21)$$

In the present work we employ the matter distribution $\rho(r) = \rho_n(r) + \rho_p(r)$, where $\rho_n(r)$ is normalized to the number of neutrons and $\rho_p(r)$ to the number of protons, so that $\rho(r)$ is normalized to the number of particles A (mass number).

6) Densities calculated within the framework of microscopic mean field approaches. Namely, densities obtained from Hartree-Fock calculations with density dependent forces of Skyrme type (DDHF) [14] and the ones using the relativistic mean field (RMF) theory [15].

We have computed the information entropy \mathcal{S} using the above densities. Our results are shown in Table 1. For the HO potential results are provided only up to ^{40}Ca , since this model is not expected to give realistic results for heavier nuclei. The results for the Skyrme and RMF theories have been obtained with the effective forces SkM* [22] and NL3 [23] respectively. It is interesting to note, however, that using different Skyrme or RMF parametrizations, we have obtained quite similar results i.e. the estimate of the entropy is independent of the used effective force in either theory.

We observe in Table 1 that \mathcal{S} increases from left to the right i.e. on going from crude to more sophisticated (microscopic) models, although this trend is less clear to the right of the table, where the value of \mathcal{S} tends to saturation. Therefore, we can

conclude that the larger \mathcal{S} , the better the quality of $\rho(r)$. It is also seen that from the various functional forms used for the description of the densities, the Fermi density shows the best behaviour leading to values for \mathcal{S} quite similar to those of the microscopic models. It is also observed that SP-D gives also large \mathcal{S} values i.e. it is a good density according to the present criterion. This is expected because SP-D reproduces fairly well the experimental data. Moreover, the \mathcal{S} values of SP-D are quite similar to those of Fermi distribution and one could say that they both lead to $\rho(r)$ of similar quality. The interesting thing is that the experimental input used for the determination of their parameters is quite different. In Fermi distribution the parameters are treated as free parameters determined by a global fit to experimental rms radii while in SP-D the parameters (not free) are adjusted to the experimental separation energies of the last proton and neutron of each nucleus.

4 An alternative approach

Gadre and Bendale (GB) [5, 6] employed a different maximum entropy procedure for atomic systems. They studied the entropy sum $\mathcal{S}_r + \mathcal{S}_k$ where

$$\mathcal{S}_r = - \int \rho(\bar{r}) \ln \rho(\bar{r}) d\bar{r} \quad (22)$$

$$\mathcal{S}_k = - \int n(\bar{k}) \ln n(\bar{k}) d\bar{k} \quad (23)$$

\mathcal{S}_r is the position-space information entropy and \mathcal{S}_k is the momentum-space information entropy. $\rho(\bar{r})$ and $n(\bar{k})$ are the single-particle densities in configuration and momentum space respectively. They found that the sum $\mathcal{S}_r + \mathcal{S}_k$ increases with the basis-set quality of the electron density $\rho(r)$.

In [9] we have focused on the same sum $\mathcal{S}_r + \mathcal{S}_k$ but for another many-fermion system i.e. the nucleus. We have employed two models of the nucleus, first the nuclear mean field was approximated by a HO potential and then the model was extended by introducing some sort of short-range correlations. In both approaches we have found that $\mathcal{S}_r + \mathcal{S}_k$ is independent of the single parameter of the model (the HO parameter) i.e. it is scale invariant and characterizes every nucleus. We have also found that short-range correlations increase slightly the net information content $\mathcal{S}_r + \mathcal{S}_k$ of the nucleus. The relative increase in $\mathcal{S}_r + \mathcal{S}_k$ due to short range correlations ranges from 2.5% for ${}^4\text{He}$ to 1.2% for ${}^{40}\text{Ca}$.

In the present work we calculate the sum $\mathcal{S}_r + \mathcal{S}_k$ for the three doubly magic nuclei ${}^4\text{He}$, ${}^{16}\text{O}$ and ${}^{40}\text{Ca}$ using as input $\rho(r)$ and $n(k)$ from a phenomenological method [24]

based on the natural orbital representation to construct the one-body density matrix (OBDM) $\rho(\bar{r}, \bar{r}')$. According to this method:

$$\begin{aligned}\rho(\bar{r}) &\equiv \rho(\bar{r}, \bar{r}) = \sum_i \lambda_i |\psi_i(\bar{r})|^2 \\ n(\bar{k}) &\equiv n(\bar{k}, \bar{k}) = \sum_i \lambda_i |\tilde{\psi}_i(\bar{k})|^2\end{aligned}\tag{24}$$

where $i = nlm$, $\tilde{\psi}_i(\bar{k})$ is the Fourier transform of $\psi_i(\bar{r})$ and λ_{nl} are the occupation numbers. The natural orbitals can be looked for in the form:

$$\psi_i(\bar{r}) \equiv \psi_{nlm}(\bar{r}) = R_{nl}(r)Y_{lm}(\theta, \phi)\tag{25}$$

The radial part of the natural orbitals of the OBDM are expanded [24] in terms of single-particle wavefunctions $\{\phi_{nl}(r)\}$ preserving all the usual symmetries for spherical nuclei:

$$R_\alpha = \sum_{i=1}^3 C_i^\alpha \phi_{il}(r) \quad (\alpha \equiv nl)\tag{26}$$

In ref. [24] three sets of s.p. wavefunctions $\{\phi_{nl}(r)\}$ were used corresponding to:

1) the harmonic oscillator potential (HO)

$$V(r) = -V_0 + \frac{1}{2}m\omega^2 r^2 \quad (V_0 > 0)\tag{27}$$

2) the square well (SW) potential with infinite walls

$$V(r) = \begin{cases} -V_0 & r < x, \\ \infty & r > x \end{cases} \quad V_0 > 0\tag{28}$$

3) the modified harmonic-oscillator (MHO) potential [25]

$$V(r) = -V_0 + \frac{1}{2}m\omega^2 r^2 + \frac{B}{r^2}, \quad V_0 > 0, B \geq 0\tag{29}$$

The parameters of the above expressions were obtained in [24] by fitting simultaneously the local density $\rho(r)$ and the momentum distribution $n(k)$ to the available empirical data. However, while for the density distribution a lot of information is available, this is not the case with the momentum distribution where the information is rather limited. Experimental data for $n(k)$ is available only for ^4He [26]. For this reason, the theoretical estimates of $n(k)$ in ^{16}O and ^{40}Ca obtained within the Jastrow correlation method (JCM) [27] were used in the fit. In all cases examined the best-fit values were obtained using the square-well single-particle wavefunctions.

5 Numerical results for the sum $\mathcal{S}_r + \mathcal{S}_k$

In table 2, we list for comparison the \mathcal{S}_r , \mathcal{S}_k and $\mathcal{S}_r + \mathcal{S}_k$ values calculated by inserting (24) into equations (22),(23) for each set of basis wavefunctions (HO, SW, MHO). It is observed that $\mathcal{S}_r + \mathcal{S}_k$ for ${}^4\text{He}$ is a maximum for the SW case, where also the best fit to the experiment is obtained. However, this is not the case for ${}^{16}\text{O}$ and ${}^{40}\text{Ca}$ nuclei where $\mathcal{S}_r + \mathcal{S}_k$ becomes maximum for the HO case. It should be noted, however, that for ${}^{16}\text{O}$ and ${}^{40}\text{Ca}$ theoretical input for $n(k)$ has been used in the fitting procedure. Moreover the theoretical $n(k)$ values obtained within JCM were calculated using as only input experimental knowledge of the density distributions.

Our results suggest that when experimental data (${}^4\text{He}$) are reproduced well, the sum $\mathcal{S}_r + \mathcal{S}_k$ is indeed a maximum, i.e. the larger $\mathcal{S}_r + \mathcal{S}_k$, the better the quality of $\rho(r)$. This also indicates that more experimental information for $n(k)$ is called for. It is also seen that in ${}^4\text{He}$ where $n(k)$ is deduced from experiment the \mathcal{S}_k value is larger in SW case than in the HO and MHO cases where the values are smaller and very close to each other.

6 Discussion and conclusions

We have presented two methods of assessing the quality of nuclear density distributions. The first method is based on the information entropy \mathcal{S} associated with phase-space distribution. It is seen that the Fermi distributions and the densities deduced from microscopic models correspond to larger information entropies i.e. they are of better quality compared to more crude models of the nucleus. It is also observed that the semiphenomenological density (SP-D) derived by reproducing the separation energies of the last nucleon and the correct asymptotic behaviour of $\rho(r)$ is of comparable quality (according to the present criterion) with Skyrme DDHF and RMF approaches. This is expected because SP-D reproduces well the empirical values for the rms radii. Another observation is that different parametrizations of Skyrme and RMF models give similar results for the information entropy \mathcal{S} . It seems that after a certain degree of sophistication of a nuclear model is reached, the information entropy no longer increases but saturates. However, such a conclusion needs more examination.

The second method examines the sum $\mathcal{S}_r + \mathcal{S}_k$ of the entropies in position and momentum space. We have used a certain phenomenological model which constructs the one-body density matrix $\rho(r, r')$. The parameters of the corresponding densities $\rho(r)$ and $n(k)$ were found by fitting simultaneously the experimental data of $\rho(r)$ and $n(k)$. For $n(k)$, however, only for ${}^4\text{He}$ some experimental input is available. Therefore, the predictions of a model (JCM) were used as an input for the rest of the cases (${}^{16}\text{O}$

and ^{40}Ca). Our study shows that for ^4He and for wavefunctions corresponding to the best quality fit (SW), among those considered, the sum $S_r + S_k$ gets its highest value. Moreover, in ^4He , where experimental input for $n(k)$ was used, the S_k value for the best quality wavefunctions is significantly larger compared with the values obtained with the use of the other wavefunctions. For ^{16}O and ^{40}Ca , however, the sum becomes maximum for HO wavefunctions which do not correspond to the best fit. This should be connected with the use of theoretical predictions for $n(k)$ due to lack of experimental information. These results, however, should be considered preliminary because a limited number of cases have been examined in the OBDM method of ref. [24], though they are in the correct direction and suggest that the MEP works, in accord with the first method of the present paper.

Table 1: The information entropy \mathcal{S} for several nuclei using various nuclear distributions (GBP approach)

| Nucleus | UN | TR | HO | SP-D | FM | DDHF | RMF |
|-------------------|---------|---------|--------|---------|---------|---------|---------|
| ^{16}O | 99.69 | 101.68 | 102.06 | 102.11 | 102.12 | 102.10 | 102.13 |
| ^{32}S | 199.38 | 202.34 | 202.75 | 202.81 | 202.88 | 202.80 | 202.90 |
| ^{40}Ca | 249.23 | 252.59 | 253.04 | 253.08 | 253.18 | 253.11 | 253.17 |
| ^{90}Zr | 560.77 | 566.10 | | 566.66 | 566.96 | 566.90 | 566.94 |
| ^{116}Sn | 722.76 | 728.68 | | 729.45 | 729.91 | 729.97 | 729.88 |
| ^{208}Pb | 1295.99 | 1304.57 | | 1304.91 | 1305.99 | 1305.81 | 1306.20 |

Table 2: The information entropies \mathcal{S}_r , \mathcal{S}_k and $\mathcal{S}_r + \mathcal{S}_k$ for three nuclei using three sets of single particle wavefunctions corresponding to harmonic oscillator (HO), square well(SW) and modified harmonic oscillator (MHO) potentials (GB approach)

| Nucleus | HO | | | SW | | | MHO | | |
|------------------|-----------------|-----------------|---------------------------------|-----------------|-----------------|---------------------------------|-----------------|-----------------|---------------------------------|
| | \mathcal{S}_r | \mathcal{S}_k | $\mathcal{S}_r + \mathcal{S}_k$ | \mathcal{S}_r | \mathcal{S}_k | $\mathcal{S}_r + \mathcal{S}_k$ | \mathcal{S}_r | \mathcal{S}_k | $\mathcal{S}_r + \mathcal{S}_k$ |
| ^4He | 7.27 | 2.06 | 9.33 | 6.91 | 4.26 | 11.17 | 7.10 | 2.28 | 9.38 |
| ^{16}O | 27.96 | 3.69 | 31.65 | 27.91 | 2.80 | 30.71 | 28.02 | 1.20 | 29.22 |
| ^{40}Ca | 66.22 | 7.82 | 74.04 | 65.67 | -5.81 | 59.86 | 66.38 | -9.09 | 57.29 |

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